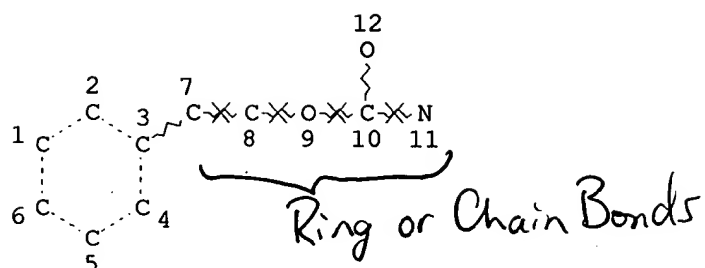


=&gt; d que 170

L13

STR



## NODE ATTRIBUTES:

CONNECT IS E1 RC AT 12

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 3

NUMBER OF NODES IS 12

## STEREO ATTRIBUTES: NONE

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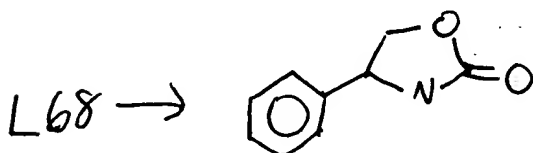
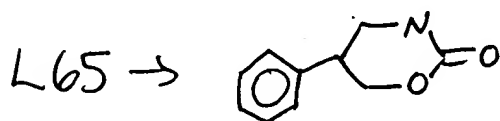
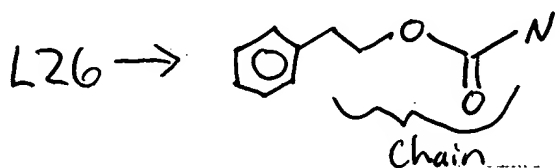
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L26 616 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND NRS<2 AND NR<2

L65 40 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND 46.220/RID

L68 744 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND NRS<3 AND NR<3 AND 16.239/RID

L70 17 SEA FILE=HCAPLUS ABB=ON PLU=ON (L65 OR L68) AND L26



L70 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 2001:490075 HCAPLUS

DN 135:204893

TI The Chemistry, Toxicology, and Identification in Rat and Human Urine of 4-Hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one: A Reactive Metabolite in Felbamate Bioactivation

AU Dieckhaus, Christine M.; Santos, Webster L.; Sofia, R. Duane; Macdonald, Timothy L.

CS Chemistry Department, University of Virginia, Charlottesville, VA, 22901, USA

SO Chem. Res. Toxicol. (2001), 14(8), 958-964

CODEN: CRTOEC; ISSN: 0893-228X

PB American Chemical Society

DT Journal

LA English

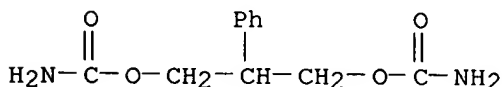
AB 4-Hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one has been proposed to be a reactive metabolite of the anti-epileptic drug felbamate. 4-Hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one exists in equil. with 3-oxo-2-phenylpropyl aminooate, which is known to eliminate to generate 2-phenylpropenal. Thus, this species is postulated to be a latent form of the ultimate reactive metabolite, 2-phenylpropenal. The chem. of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one is proposed to parallel that of 4-hydroxycyclophosphamide, the bioactivated form of cyclophosphamide that undergoes ring-opening to aldophosphamide and subsequent elimination to afford 2-propenal (acrolein). The work presented here reports the chem. synthesis of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one and demonstrates that under buffered conditions it exists in equil. with 3-oxo-2-phenylpropyl aminooate. The rate-limiting step in the decompn. of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one is the irreversible .beta.-elimination from 3-oxo-2-phenylpropyl aminooate to 2-phenylpropenal. We have found the half-life of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one to be 4.6.+-.0.4 h under in vitro conditions that mimic the physiol. setting. As a consequence of the relatively long half-life of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one, we have sought evidence for the significance of this pathway in exptl. and clin. conditions. We report here the observation of this metabolite in the urine of rats being treated with 3-hydroxy-2-phenylpropyl aminooate, the esterase-mediated metabolite of felbamate, and in the urine of patients undergoing felbamate therapy. In addn., we have shown that 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one is toxic to cultured cells in a time-dependent manner, most likely as a result of its decompn. to 2-phenylpropenal. Taken together, the data support the hypothesis that 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one represents a "time-release" form of 2-phenylpropenal capable of traveling to distal sites from its locus of bioactivation and thereby mediates felbamate assocd. toxicities.

IT 25451-15-4, Felbamate

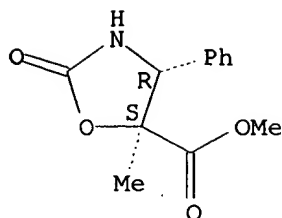
RL: BPR (Biological process); BIOL (Biological study); PROC (Process) (chem., toxicol., and identification in rat and human urine of a reactive metabolite in felbamate bioactivation)

RN 25451-15-4 HCAPLUS

CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



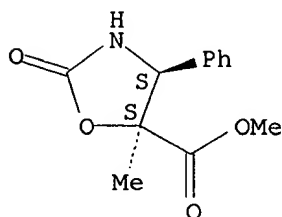
2 of 4  
Inventors



RN 335200-12-9 HCAPLUS

CN 5-Oxazolidinecarboxylic acid, 5-methyl-2-oxo-4-phenyl-, methyl ester,  
(4S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 65

RE

(1) Ager, D; Aldrichimica Acta 1997, V30, P3 HCAPLUS

(2) Ager, D; Chem Rev 1996, V96, P835 HCAPLUS

(3) Albone, D; J Org Chem 1998, V63, P9569 HCAPLUS

(4) Au, S; Chem Commun 1998, P2677 HCAPLUS

(5) Au, S; J Am Chem Soc 1999, V121, P9120 HCAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 2000:573661 HCAPLUS

DN 133:172201

TI Felbamate derived compounds

IN MacDonald, Timothy L.; Miller, Thomas A.; Thompson, Charles D.

PA University of Virginia Patent Foundation, USA

SO PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DT Patent

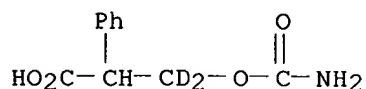
LA English

FAN.CNT 1

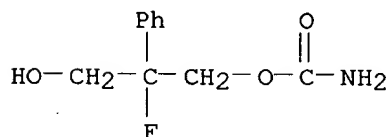
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000047202	A1	20000817	WO 2000-US3147	20000208
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,				

3 of 4  
← Inventors  
Applied

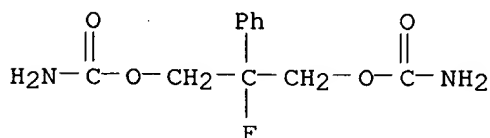
RN 288302-37-4 HCAPLUS  
 CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl-d2]- (9CI) (CA INDEX NAME)



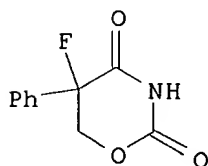
IT 288302-42-1P  
 RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)  
 RN 288302-42-1 HCAPLUS  
 CN 1,3-Propanediol, 2-fluoro-2-phenyl-, monocarbamate (9CI) (CA INDEX NAME)

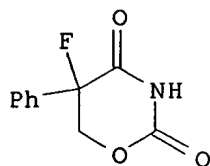


IT 726-99-8P 288302-44-3P  
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)  
 RN 726-99-8 HCAPLUS  
 CN 1,3-Propanediol, 2-fluoro-2-phenyl-, dicarbamate (9CI) (CA INDEX NAME)



RN 288302-44-3 HCAPLUS  
 CN 2H-1,3-Oxazine-2,4(3H)-dione, 5-fluorodihydro-5-phenyl- (9CI) (CA INDEX NAME)





IT 25451-15-4D, Felbamate, derivs. 288302-40-9

288302-41-0

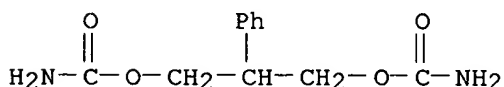
RL: BAC (Biological activity or effector, except adverse); THU

(Therapeutic use); BIOL (Biological study); USES (Uses)

(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)

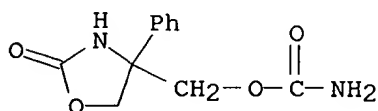
RN 25451-15-4 HCAPLUS

CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



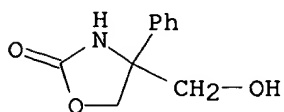
RN 288302-40-9 HCAPLUS

CN 2-Oxazolidinone, 4-[[ (aminocarbonyl)oxy]methyl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 288302-41-0 HCAPLUS

CN 2-Oxazolidinone, 4-(hydroxymethyl)-4-phenyl- (9CI) (CA INDEX NAME)



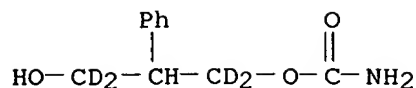
IT 288302-36-3P 288302-43-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)

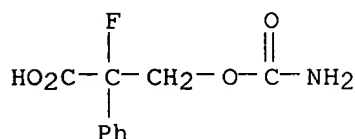
RN 288302-36-3 HCAPLUS

CN 1,3-Propane-1,1,3,3-d4-diol, 2-phenyl-, monocarbamate (9CI) (CA INDEX NAME)



RN 288302-43-2 HCAPLUS

CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl]-.alpha.-fluoro-(9CI) (CA INDEX NAME)



RE.CNT 2

RE

(1) Choi; 1987, 2, P705 HCAPLUS

(2) Choi; Tetrahedron 1986, V42(23), P6399 HCAPLUS

L70 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 2000:213938 HCAPLUS

DN 132:342749

TI The synthesis, in vitro reactivity, and evidence for formation in humans of 5-phenyl-1,3-oxazinane-2,4-dione, a metabolite of felbamate

AU Thompson, Charles D.; Miller, Thomas A.; Barthen, Mary T.; Dieckhaus, Christine M.; Sofia, R. Duane; Macdonald, Timothy L.

CS Chemistry Department, University of Virginia, Charlottesville, VA, 22901, USA

SO Drug Metab. Dispos. (2000), 28(4), 434-439

CODEN: DMDSAI; ISSN: 0090-9556

PB American Society for Pharmacology and Experimental Therapeutics

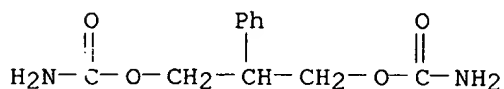
DT Journal

LA English

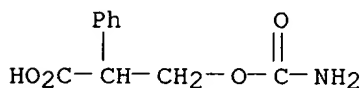
AB Previously we have proposed and provided evidence for a metabolic scheme leading to 3-carbamoyl-2-phenylpropionaldehyde from the antiepileptic drug felbamate. This aldehyde was found to undergo reversible cyclization to form the more stable cyclic carbamate 4-hydroxy-5-phenyl-tetrahydro-1,3-oxazin-2-one or undergo elimination to form 2-phenylpropenal. The cyclic carbamate bears structural similarity to 4-hydroxycyclophosphamide and there is an intriguing parallelism between the pathway from the cyclic carbamate to 2-phenylpropenal and the known pathway from 4-hydroxycyclophosphamide to acrolein. The similarity of these transformations led us to consider 5-phenyl-1,3-oxazinane-2,4-dione, which could arise from an oxidn. of the cyclic carbamate, as a potential metabolite of felbamate. As the formation of this dione species may have both potential pharmacol. and toxicol. implications for felbamate therapy, we wished to study its reactivity. We have developed a synthesis of 5-phenyl-1,3-oxazinane-2,4-dione and evaluated its reactivity in vitro. This dione was found to undergo base-catalyzed decompn. to three products, one of which is the major human metabolite of felbamate, 3-carbamoyl-2-phenylpropionic acid. Furthermore, we have found evidence for the presence of the dione in human urine after felbamate treatment through the identification of its major in vitro decompn. product, 2-phenylacrylamide 11.

All 4  
Inventors

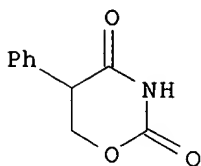
IT **25451-15-4, Felbamate**  
 RL: BPR (Biological process); BIOL (Biological study); PROC (Process)  
 (synthesis, in vitro reactivity, and evidence for formation in humans  
 of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)  
 RN 25451-15-4 HCAPLUS  
 CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



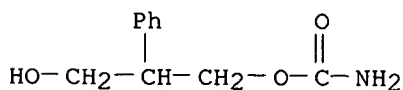
IT **139262-66-1P**  
 RL: FMU (Formation, unclassified); RCT (Reactant); SPN (Synthetic  
 preparation); FORM (Formation, nonpreparative); PREP (Preparation)  
 (synthesis, in vitro reactivity, and evidence for formation in humans  
 of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)  
 RN 139262-66-1 HCAPLUS  
 CN Benzeneacetic acid, .alpha.-[[[aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX  
 NAME)

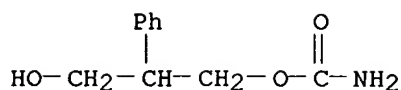


IT **269062-79-5P**  
 RL: MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic  
 preparation); BIOL (Biological study); FORM (Formation, nonpreparative);  
 PREP (Preparation)  
 (synthesis, in vitro reactivity, and evidence for formation in humans  
 of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)  
 RN 269062-79-5 HCAPLUS  
 CN 2H-1,3-Oxazine-2,4(3H)-dione, dihydro-5-phenyl- (9CI) (CA INDEX NAME)



IT **25451-53-0**  
 RL: RCT (Reactant)  
 (synthesis, in vitro reactivity, and evidence for formation in humans  
 of felbamate metabolite 5-phenyl-1,3-oxazinane-2,4-dione)  
 RN 25451-53-0 HCAPLUS  
 CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)





RE.CNT 12

RE

- (1) Adusumalli, V; Drug Metab Dispos 1993, V21, P710 HCAPLUS
- (2) Kapetanovic, I; Drug Metab Dispos 1998, V26, P1089 HCAPLUS
- (5) Takamizawa, A; Chem Pharm Bull (Tokyo) 1972, V20, P1612 HCAPLUS
- (6) Testa, E; J Org Chem 1959, V24, P1928 HCAPLUS
- (7) Thompson, C; Chem Res Toxicol 1996, V9, P1225 HCAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1998:725893 HCAPLUS

DN 130:104748

TI Potentially reactive cyclic carbamate metabolite of the antiepileptic drug / felbamate produced by human liver tissue in vitro

AU Kapetanovic, Izet M.; Torchin, Cynthia D.; Thompson, Charles D.; Miller, Thomas A.; McNeilly, Patrick J.; MacDonald, Timothy L.; Kupferberg, Harvey J.; Perhach, James L.; Sofia, R. Duane; Strong, John M.

CS Epilepsy Branch, National Institute of Neurological Disorders and Stroke, USA

SO Drug Metab. Dispos. (1998), 26(11), 1089-1095

CODEN: DMDSAI; ISSN: 0090-9556

PB Lippincott Williams &amp; Wilkins

DT Journal

LA English

AB Felbamate (FBM) is a novel antiepileptic drug that was approved in 1993 for treatment of several forms of epilepsy. After its introduction, toxic reactions (aplastic anemia and hepatotoxicity) assocd. with its use were reported. It is unknown whether FBM or one of its metabolites is responsible for these idiosyncratic adverse reactions. Although the metab. of FBM has not been fully characterized, three primary metabolites of FBM have been identified, i.e. 2-hydroxy, p-hydroxy, and monocarbamate metabolites. In addn., the monocarbamate metabolite leads to a carboxylic acid, which is the major metabolite of FBM in humans. Formation of the hydroxylated products of FBM involves cytochrome P 450 enzymes, but the enzymes involved in the formation and further metab. of the monocarbamate have not yet been elucidated. Recently, mercapturate metabolites of FBM have been identified in human urine, and a metabolic scheme involving reactive aldehyde metabolite formation from the monocarbamate metabolite has been proposed. The present study confirmed the formation of the proposed metabolites using human liver tissue in vitro. The aldehyde intermediates were trapped as oxime derivs., and the cyclic equil. product (proposed as a storage and transport form for the aldehydes) was monitored directly by HPLC or GC/MS. Formation of putative toxic aldehyde intermediates and the major carboxylic acid metabolite of FBM was differentially effected with the cofactors NADP+ and NAD+. It is possible that the cofactors may influence the relative metab. via activation and inactivation pathways.

IT 25451-15-4, Felbamate 25451-53-0, 2-Phenyl-1,3-propanediol monocarbamate

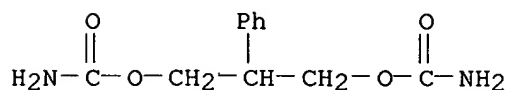
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)

(potentially reactive cyclic carbamate metabolite of the antiepileptic drug felbamate produced by human liver tissue in vitro)

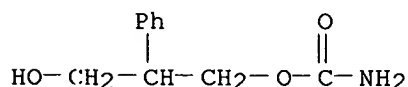
3 of 4



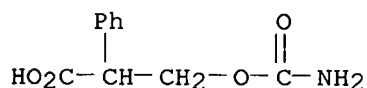
RN 25451-15-4 HCAPLUS  
 CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)



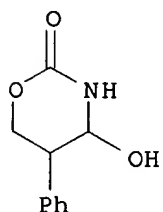
RN 25451-53-0 HCAPLUS  
 CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)



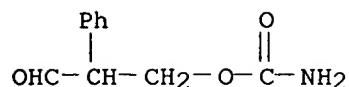
IT 139262-66-1 183961-08-2  
 RL: MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
 (potentially reactive cyclic carbamate metabolite of the antiepileptic drug felbamate produced by human liver tissue in vitro)  
 RN 139262-66-1 HCAPLUS  
 CN Benzeneacetic acid, .alpha.-[[ (aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX NAME)



RN 183961-08-2 HCAPLUS  
 CN 2H-1,3-Oxazin-2-one, tetrahydro-4-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)



IT 183961-07-1  
 RL: MFM (Metabolic formation); RCT (Reactant); BIOL (Biological study); FORM (Formation, nonpreparative)  
 (potentially reactive cyclic carbamate metabolite of the antiepileptic drug felbamate produced by human liver tissue in vitro)  
 RN 183961-07-1 HCAPLUS  
 CN Benzeneacetaldehyde, .alpha.-[[ (aminocarbonyl)oxy]methyl]- (9CI) (CA INDEX NAME)



RE.CNT 17

RE

- (1) Adusumalli, V; Drug Metab Dispos 1993, V21, P710 HCAPLUS
- (2) Anderson, L; J Chromatogr 1995, V667, P247 HCAPLUS
- (3) Glue, P; Clin Pharmacokine 1997, V33, P214 HCAPLUS
- (4) Guengerich, F; Chem Res Toxicol 1991, V4, P413 HCAPLUS
- (5) Ingelman-Sundberg, M; Exper Suppl 1994, V71, P197 HCAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1996:664849 HCAPLUS

DN 126:300

TI Synthesis and in Vitro Reactivity of 3-Carbamoyl-2-phenylpropionaldehyde  
and 2-Phenylpropenal: Putative Reactive Metabolites of Felbamate

AU Thompson, Charles D.; Kinter, Michael T.; Macdonald, Timothy L.

CS Chemistry Department, University of Virginia, Charlottesville, VA, 22901,  
USA

SO Chem. Res. Toxicol. (1996), 9(8), 1225-1229

CODEN: CRTOEC; ISSN: 0893-228X

PB American Chemical Society

DT Journal

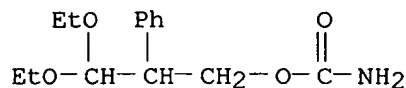
LA English

AB We propose that 3-carbamoyl-2-phenylpropionaldehyde is an intermediate in the metab. of felbamate, an anti-epileptic drug with a unique profile of therapeutic activity, and undergoes a cascade of chem. reactions responsible for the toxic properties of the parent drug. To test this hypothesis, we have synthesized 3-carbamoyl-2-phenylpropionaldehyde and evaluated its in vitro reactivity. This mol. was found to be highly unstable at physiol. pH (t1/2 .ltoreq. 30 s) and to undergo facile elimination to 2-phenylpropenal, an .alpha.,.beta.-unsatd. aldehyde commonly termed atropaldehyde. However, the predominant reaction pathway for 3-carbamoyl-2-phenylpropionaldehyde was reversible cyclization to generate 4-hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one, a urethane that has a considerably longer half-life at physiol. pH (t1/2 .gtoreq. 5 h) and may serve as a stable reservoir of the reactive aldehyde both in vitro and in vivo. Atropaldehyde is a potent electrophile and was found to exhibit cytotoxicity to cultured fibroblasts (50% growth inhibition (GI50) = 4.1 .+- .1.1 .mu.M) comparable to the known unsatd. aldehyde toxins, 4-hydroxy-2-nonenal and acrolein. 3-Carbamoyl-2-phenylpropionaldehyde also exhibited significant cytotoxicity (GI50 = 53 .+- .8 .mu.M), whereas 2-phenyl-1,3-propanediol monocarbamate (GI50 > 500 .mu.M) and 3-carbamoyl-2-phenylpropionic acid (GI50 > 500 .mu.M) were nontoxic. We have addnl. demonstrated the formation of a glutathione-atropaldehyde conjugate from the in vitro incubation of 3-carbamoyl-2-phenylpropionaldehyde with glutathione. Thus, the potent cytotoxicity and potential allergenicity of atropaldehyde implicate this unsatd. aldehyde as a possible causative agent in the toxicities obsd. with felbamate treatment.

IT 183961-10-6P

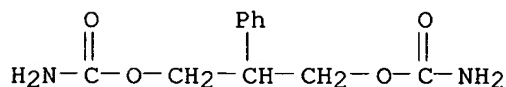
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(intermediate; synthesis and in vitro reactivity of putative toxic  
metabolites of felbamate)

RN 183961-10-6 HCAPLUS  
 CN Benzeneethanol, .beta.-(diethoxymethyl)-, carbamate (9CI) (CA INDEX NAME)



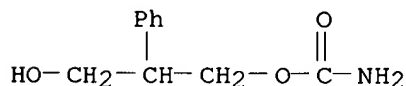
IT 25451-15-4, Felbamate  
 RL: ADV (Adverse effect, including toxicity); BPR (Biological process);  
 BIOL (Biological study); PROC (Process)  
 (synthesis and in vitro reactivity of putative toxic metabolites of  
 felbamate)

RN 25451-15-4 HCAPLUS  
 CN 1,3-Propanediol, 2-phenyl-, dicarbamate (8CI, 9CI) (CA INDEX NAME)

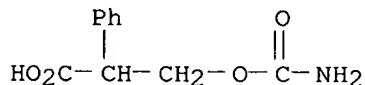


IT 25451-53-0, 2-Phenyl-1,3-propanediol monocarbamate  
 139262-66-1  
 RL: ADV (Adverse effect, including toxicity); MFM (Metabolic formation);  
 BIOL (Biological study); FORM (Formation, nonpreparative)  
 (synthesis and in vitro reactivity of putative toxic metabolites of  
 felbamate)

RN 25451-53-0 HCAPLUS  
 CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)

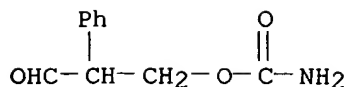


RN 139262-66-1 HCAPLUS  
 CN Benzeneacetic acid, .alpha.-[[[aminocarbonyl]oxy]methyl]- (9CI) (CA INDEX NAME)



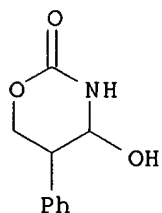
IT 183961-07-1P 183961-08-2P  
 RL: MFM (Metabolic formation); SPN (Synthetic preparation); BIOL  
 (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)  
 (synthesis and in vitro reactivity of putative toxic metabolites of  
 felbamate)

RN 183961-07-1 HCAPLUS  
 CN Benzeneacetaldehyde, .alpha.-[[[aminocarbonyl]oxy]methyl]- (9CI) (CA INDEX NAME)



RN 183961-08-2 HCAPLUS

CN 2H-1,3-Oxazin-2-one, tetrahydro-4-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)



L70 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1991:428963 HCAPLUS

DN 115:28963

TI Synthesis, conformation, crystal structures and DNA cleavage abilities of tetracyclic analogs of quinocarcin

AU Williams, Robert M.; Glinka, Tomasz; Gallegos, Renee; Ehrlich, Paul P.; Flanagan, Mark E.; Coffman, Hazel; Park, Gyoosoon

CS Dep. Chem., Colorado State Univ., Fort Collins, CO, 80523, USA

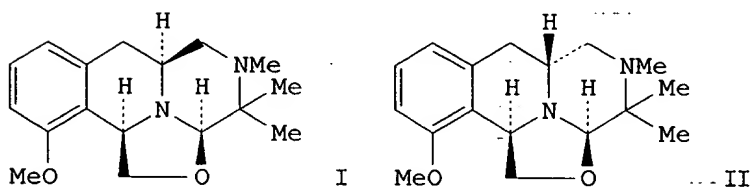
SO Tetrahedron (1991), 47(14-15), 2629-42

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

GI



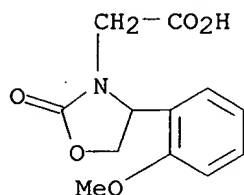
AB Racemic tetracyclic quinocarcin analogs I and II were prepd. and their DNA cleaving abilities investigated. Both substances effect the modest cleavage of plasmid DNA. Alteration of the conformation of the reactive oxazolidine fused to the piperazine ring by selecting the stereochem. at C-11a drastically attenuated the relative ability of these substances to cleave DNA.

IT 108343-93-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and intramol. acylation of, isoquinoline from)

RN 108343-93-7 HCAPLUS

CN 3-Oxazolidineacetic acid, 4-(2-methoxyphenyl)-2-oxo- (9CI) (CA INDEX NAME)

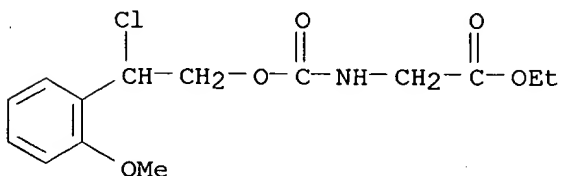


IT 134307-60-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and intramol. cyclocondensation of, oxazole from)

RN 134307-60-1 HCAPLUS

CN Glycine, N-[[2-chloro-2-(2-methoxyphenyl)ethoxy]carbonyl]-, ethyl ester  
(9CI) (CA INDEX NAME)



L70 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1990:669 HCAPLUS

DN 112:669

TI Amino acid derivatives, processes for their preparation, and  
pharmaceutical compositions comprising them for treatment of hypertension  
and heart failure

IN Hemmi, Keiji; Neya, Masahiro; Marusawa, Hiroshi; Imai, Keisuke; Kayakiri,  
Natsuko; Hashimoto, Masashi

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO Eur. Pat. Appl., 60 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 300189	A2	19890125	EP 1988-109430	19880614
	EP 300189	A3	19900822		
	EP 300189	B1	19941102		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ZA 8804087	A	19890222	ZA 1988-4087	19880608
	US 4921855	A	19900501	US 1988-204549	19880609
	ES 2067456	T3	19950401	ES 1988-109430	19880614
	FI 8802875	A	19881223	FI 1988-2875	19880616
	FI 96202	B	19960215		
	FI 96202	C	19960527		
	IL 86782	A1	19930404	IL 1988-86782	19880616

AU 8818190	A1	19881222	AU 1988-18190	19880621
AU 617674	B2	19911205		
DK 8803400	A	19881223	DK 1988-3400	19880621
NO 8802732	A	19881223	NO 1988-2732	19880621
NO 175371	B	19940627		
NO 175371	C	19941005		
CN 1030411	A	19890118	CN 1988-103878	19880621
CN 1026892	B	19941207		
JP 01019071	A2	19890123	JP 1988-153041	19880621
JP 06025147	B4	19940406		
HU 47917	A2	19890428	HU 1988-3164	19880621
HU 202212	B	19910228		
SU 1801107	A3	19930307	SU 1988-4356019	19880621
US 5142048	A	19920825	US 1990-462117	19900108
RU 2070195	C1	19961210	RU 1991-5010142	19911122
US 5223489	A	19930629	US 1992-828193	19920130
PRAI GB 1987-14597		19870622		
GB 1987-25511		19871030		
GB 1988-5389		19880307		
US 1988-204549		19880609		
US 1990-462117		19900108		

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A process for prepg. I [R1 = lower alkyl optionally substituted with acyl, hydroxy, lower alkoxy, aryl, lower alkylthio, NR5R6; R5 = H, acyl; R6 = H, lower alkyl, aryl, (lower alkyl- or acyl-substituted) amino; R2, R3 = H, lower alkyl; R4 = lower alkyl; R1NR2 = heterocycle optionally substituted with lower alkyl, hydroxy(lower)alkyl, lower alkoxy(lower)alkyl, acyl(lower)alkyl, oxo, acyl] or its pharmaceutically acceptable salt comprises (a) reacting II (R3, R4 as above; R8 = H, N-protective group) or its reactive deriv. at the amino group or a salt thereof with III (R1, R2 as above) or its reactive deriv. at the COO group or a salt thereof, and, if necessary, eliminating the N-protective group or (b) subjecting IV (R2, R3, R4, R6 as above; R7 = N-protective group; A = lower alkylene) or its salt to elimination reaction of R7 to give V (R2, R3, R4, R6, A as above) or its salt. I are useful as antihypertensives or for the treatment of heart failure. A soln. of 2(S)-[N-(2-morpholinocarbonylethyl)-N-methylaminocarbonyloxy]-3-phenylpropionic acid (prepn. described) 449 and 2(S)-(N.alpha.-methyl-Nim-tosyl-L-histidyl)amino-1-cyclohexyl-3(S)-hydroxy-6-methylheptane (prepn. described) 300 mg in CH2Cl2 (30 mL) was mixed with N-ethyl-N'-(3-dimethylaminopropyl)carbodiimide-HCl 140 mg at 5.degree. overnight. The residue was dissolved in EtOAc, washed with HCl/NaHCO3, dried, redissolved in DMF, and reacted with pyridine-HCl 650 mg for 2 h at room temp. Workup and purifn. by TLC yielded 2(S)-[N.alpha.-[2(S)-[N-(2-morpholinocarbonylethyl)-N-methylaminocarbonyloxy]-3-phenylpropionyl]-N.alpha.-methyl-L-histidyl]amino-1-cyclohexyl-3(S)-hydroxy-6-methylheptane (VI) 221 mg (m.p. 80-87.degree.) as an amorphous powder. VI, dissolved in HCl and orally administered to Na-depleted male or female cynomolgus monkeys (32 mg/kg), reduced mean arterial blood pressure and plasma renin activity by 18 and 92%, resp.

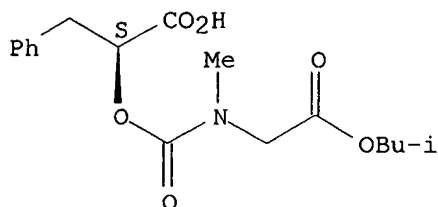
IT 124074-67-5P 124074-69-7P 124074-70-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, in antihypertensive amino acid deriv. prepn.)

RN 124074-67-5 HCAPLUS

CN Glycine, N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-, 2-methylpropyl ester, (S)- (9CI) (CA INDEX NAME)

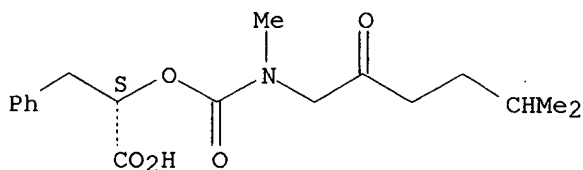
Absolute stereochemistry.



RN 124074-69-7 HCAPLUS

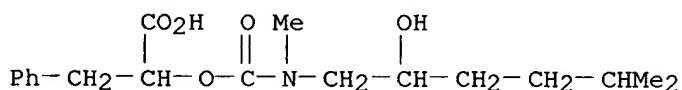
CN Benzenepropanoic acid, .alpha.-[[[methyl(5-methyl-2-oxohexyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 124074-70-0 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[(2-hydroxy-5-methylhexyl)methylamino]carbonyl]oxy]- (9CI) (CA INDEX NAME)



IT 124074-43-7P 124074-44-8P 124074-45-9P  
 124074-46-0P 124074-48-2P 124074-51-7P  
 124074-57-3P 124074-59-5P 124074-60-8P  
 124074-71-1P 124074-72-2P 124074-79-9P  
 124074-82-4P 124074-84-6P 124074-86-8P  
 124074-87-9P 124074-89-1P 124074-90-4P  
 124074-93-7P 124074-96-0P 124074-97-1P  
 124074-98-2P 124075-01-0P 124075-02-1P  
 124075-05-4P 124075-08-7P 124075-09-8P  
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 124122-51-6P

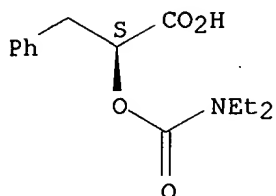
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, in prepn. of antihypertensives)

RN 124074-43-7 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[(diethylamino)carbonyl]oxy]-, (S)- (9CI)  
 (CA INDEX NAME)

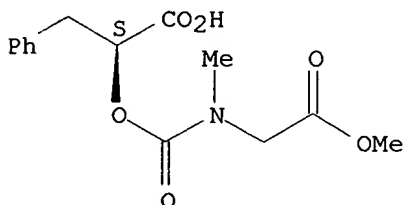
Absolute stereochemistry.



RN 124074-44-8 HCAPLUS

CN Glycine, N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-, methyl ester, (S)- (9CI) (CA INDEX NAME)

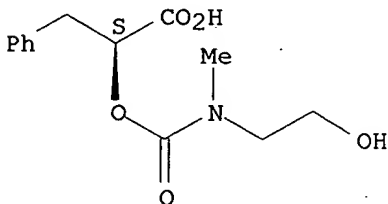
Absolute stereochemistry.



RN 124074-45-9 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[(2-hydroxyethyl)methylamino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

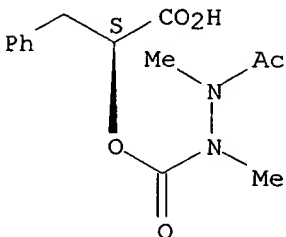
Absolute stereochemistry.



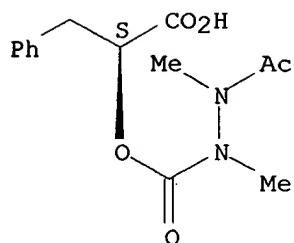
RN 124074-46-0 HCAPLUS

CN Hydrazinecarboxylic acid, 2-acetyl-1,2-dimethyl-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



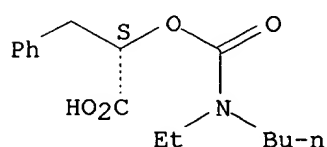




RN 124074-48-2 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[ (butylethylamino) carbonyl]oxy]-, (S)-  
(9CI) (CA INDEX NAME)

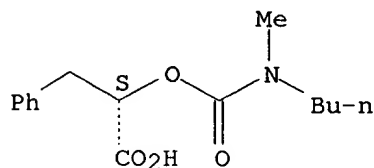
Absolute stereochemistry.



RN 124074-51-7 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[ (butylmethylamino) carbonyl]oxy]-, (S)-  
(9CI) (CA INDEX NAME)

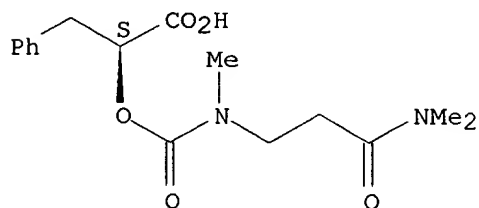
Absolute stereochemistry.



RN 124074-57-3 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[3-(dimethylamino)-3-oxopropyl]methylamino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

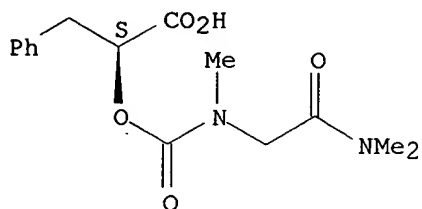
Absolute stereochemistry.



RN 124074-59-5 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[2-(dimethylamino)-2-oxoethyl]methylamino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

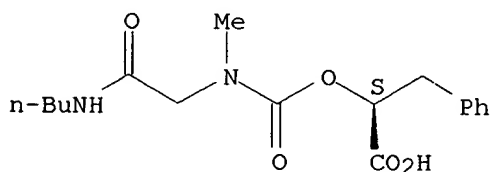
Absolute stereochemistry.



RN 124074-60-8 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[2-(butylamino)-2-oxoethyl]methylamino]carbonyloxy]-, (S)- (9CI) (CA INDEX NAME)

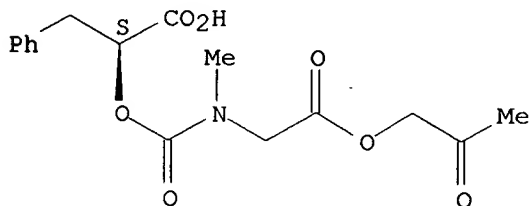
Absolute stereochemistry.



RN 124074-71-1 HCAPLUS

CN Glycine, N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-, 2-oxopropyl ester, (S)- (9CI) (CA INDEX NAME)

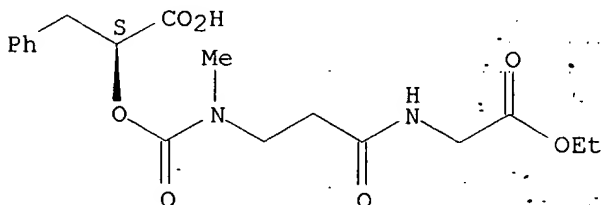
Absolute stereochemistry.



RN 124074-72-2 HCAPLUS

CN Glycine, N-[N-[(1-carboxy-2-phenylethoxy)carbonyl]-N-methyl-.beta.-alanyl]-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

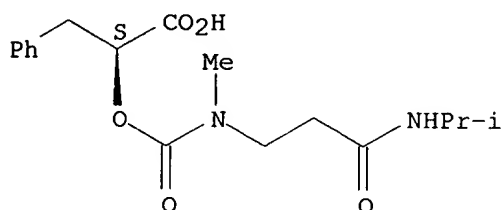


RN 124074-79-9 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(1-methylethyl)amino]-3-

oxopropyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

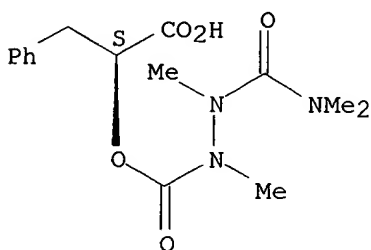
Absolute stereochemistry.



RN 124074-82-4 HCAPLUS

CN Hydrazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-1,2-dimethyl-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

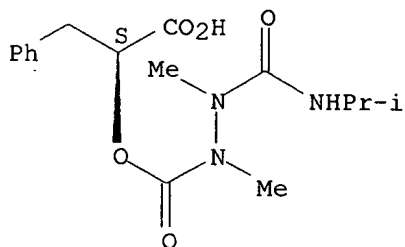
Absolute stereochemistry.



RN 124074-84-6 HCAPLUS

CN Hydrazinecarboxylic acid, 1,2-dimethyl-2-[[[(1-methylethyl)amino]carbonyl]-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

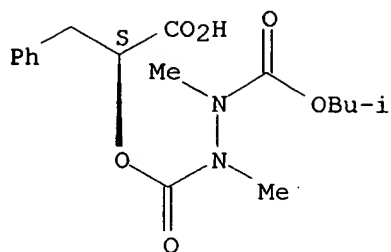
Absolute stereochemistry.



RN 124074-86-8 HCAPLUS

CN 1,2-Hydrazinedicarboxylic acid, 1,2-dimethyl-, 1-carboxy-2-phenylethyl 2-methylpropyl ester, (S)- (9CI) (CA INDEX NAME)

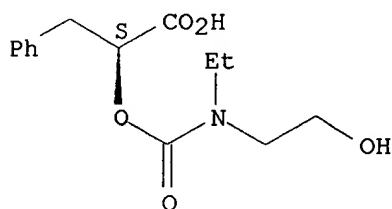
Absolute stereochemistry.



RN 124074-87-9 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[ethyl(2-hydroxyethyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

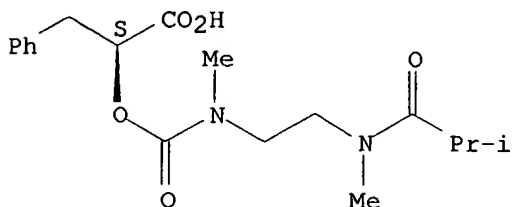
Absolute stereochemistry.



RN 124074-89-1 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl{2-[methyl(2-methyl-1-oxopropyl)amino]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

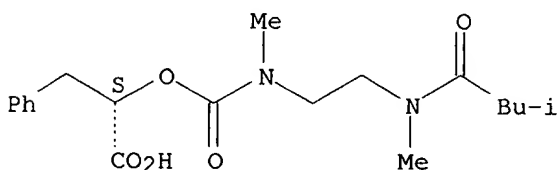
Absolute stereochemistry.



RN 124074-90-4 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl{2-[methyl(3-methyl-1-oxobutyl)amino]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

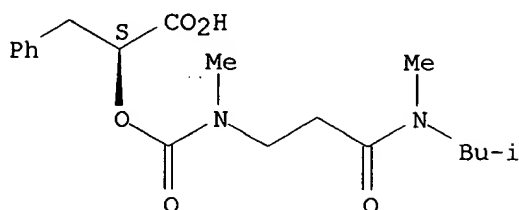


RN 124074-93-7 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl{3-[methyl(2-methylpropyl)amino]-3-

oxopropyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

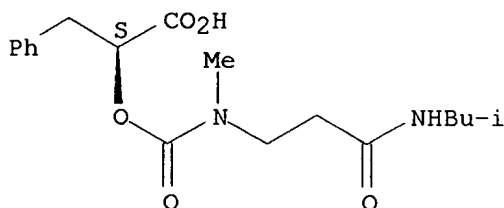
Absolute stereochemistry.



RN 124074-96-0 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(2-methylpropyl)amino]-3-oxopropyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)...

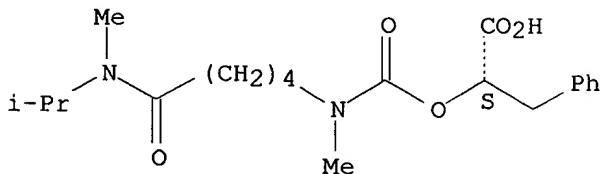
Absolute stereochemistry.



RN 124074-97-1 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl[5-[methyl(1-methylethyl)amino]-5-oxopentyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

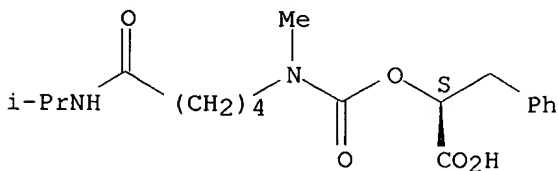
Absolute stereochemistry.



RN 124074-98-2 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl[5-[(1-methylethyl)amino]-5-oxopentyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

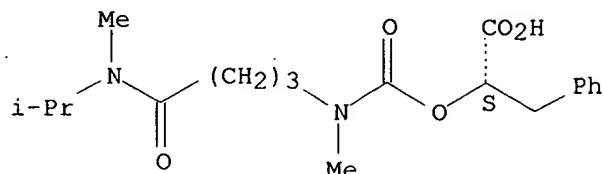
Absolute stereochemistry.



RN 124075-01-0 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl[4-[methyl(1-methylethyl)amino]-4-oxobutyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

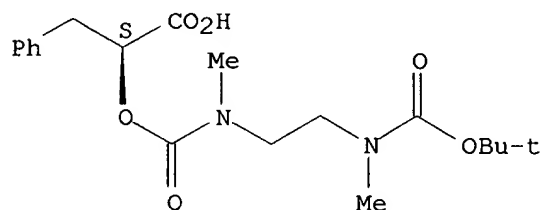
Absolute stereochemistry.



RN 124075-02-1 HCAPLUS

CN 3,10-Dioxa-5,8-diazadodecanoic acid, 5,8,11,11-tetramethyl-4,9-dioxo-2-(phenylmethyl)-, (S)- (9CI) (CA INDEX NAME)

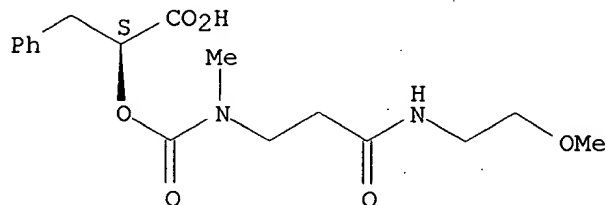
Absolute stereochemistry.



RN 124075-05-4 HCAPLUS

CN 2,11-Dioxa-5,9-diazatridecan-13-oic acid, 9-methyl-6,10-dioxo-12-(phenylmethyl)-, (S)- (9CI) (CA INDEX NAME)

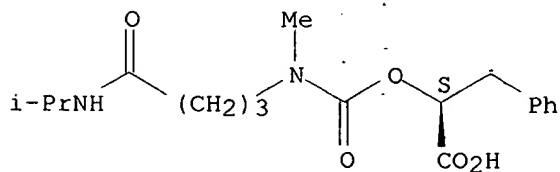
Absolute stereochemistry.



RN 124075-08-7 HCAPLUS

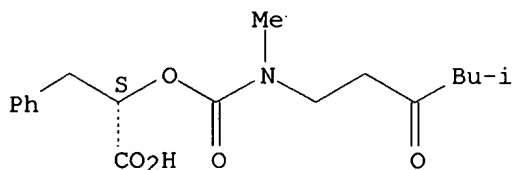
CN Benzenepropanoic acid, .alpha.-[[[methyl[4-[(1-methylethyl)amino]-4-oxobutyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



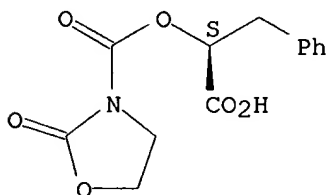
RN 124075-09-8 HCAPLUS  
 CN Benzenepropanoic acid, .alpha.-[[[methyl(5-methyl-3-oxohexyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



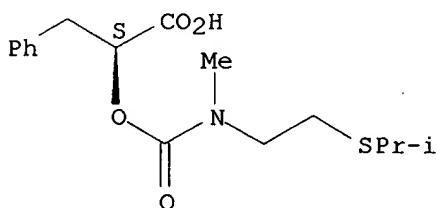
RN 124075-28-1 HCAPLUS  
 CN 3-Oxazolidinecarboxylic acid, 2-oxo-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



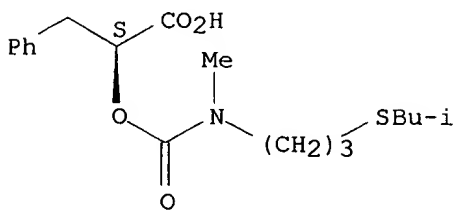
RN 124075-33-8 HCAPLUS  
 CN Benzenepropanoic acid, .alpha.-[[[methyl[2-[(1-methylethyl)thio]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

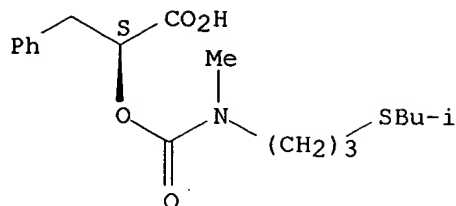
Absolute stereochemistry.



RN 124075-36-1 HCAPLUS  
 CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(2-methylpropyl)thio]propyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

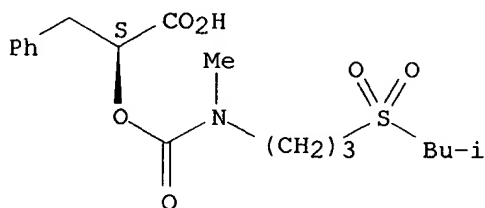




RN 124075-37-2 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl[3-[(2-methylpropyl)sulfonyl]propyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

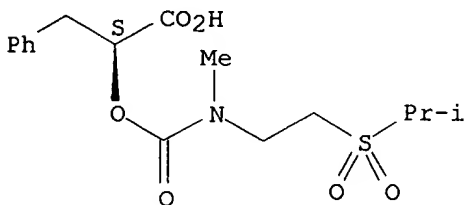
Absolute stereochemistry.



RN 124075-38-3 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[methyl[2-[(1-methylethyl)sulfonyl]ethyl]amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

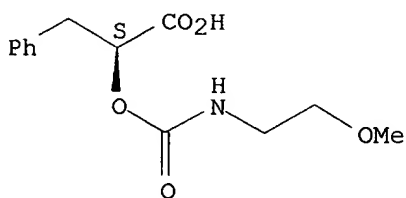
Absolute stereochemistry.



RN 124122-50-5 HCAPLUS

CN Benzenepropanoic acid, .alpha.-[[[(2-methoxyethyl)amino]carbonyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

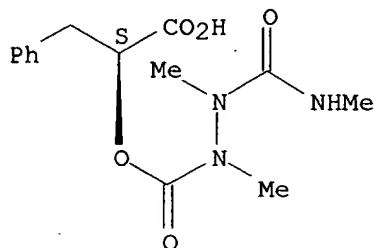


RN 124122-51-6 HCAPLUS



CN Hydrazinecarboxylic acid, 1,2-dimethyl-2-[(methylamino)carbonyl]-, 1-carboxy-2-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7C ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1988:630222 HCAPLUS

DN 109:230222

TI Diastereoconversion of threo 2-amino alcohols to erythro isomers through a new cyclocarbamation

AU Kano, Shinzo; Yuasa, Yoko; Yokomatsu, Tsutomu; Shibuya, Shiroshi

CS Tokyo Coll. Pharm., Tokyo, 192-03, Japan

SO Heterocycles (1988), 27(5), 1241-8

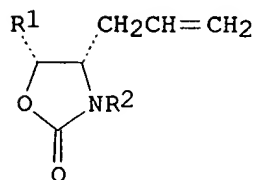
CODEN: HTCYAM; ISSN: 0385-5414

DT Journal

LA English

OS CASREACT 109:230222

GI



I

AB Amino alcs. threo-R1CH(OH)CH(NHR2)CH2CH:CH2 (R1 = Me, Me2CHCH2, PhCH2; R2 = Pr, PhCH2, Me, Et) were protected by (Me3CO)2CO, and the products were treated with SOCl2 to give oxazolidinones I. I are synthetic equiv. of erythro-R1CH(OH)CH(NHR2)CH2CH:CH2.

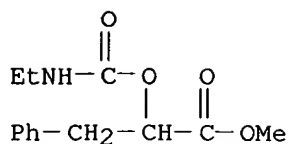
IT 117508-46-0P 117508-53-9P 117508-54-0P

117508-55-1P 117543-44-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and allylation of, by allylsilane deriv.)

RN 117508-46-0 HCAPLUS

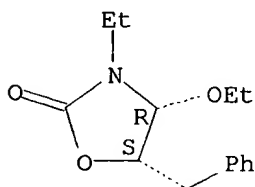
CN Benzenepropanoic acid, .alpha.-[[(ethylamino)carbonyl]oxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 117508-53-9 HCAPLUS

CN 2-Oxazolidinone, 4-ethoxy-3-ethyl-5-(phenylmethyl)-, cis- (9CI) (CA INDEX NAME)

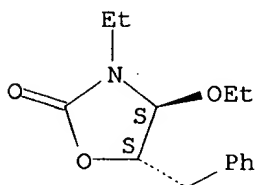
Relative stereochemistry.



RN 117508-54-0 HCAPLUS

CN 2-Oxazolidinone, 4-ethoxy-3-ethyl-5-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

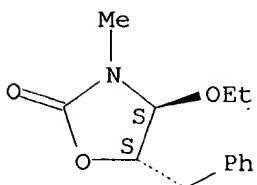
Relative stereochemistry.



RN 117508-55-1 HCAPLUS

CN 2-Oxazolidinone, 4-ethoxy-3-methyl-5-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

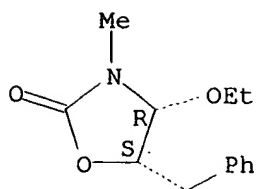
Relative stereochemistry.



RN 117543-44-9 HCAPLUS

CN 2-Oxazolidinone, 4-ethoxy-3-methyl-5-(phenylmethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

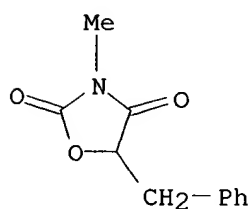


IT 5841-65-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and conversion of, to ethoxyoxazolidinone analog)

RN 5841-65-6 HCAPLUS

CN 2,4-Oxazolidinedione, 3-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



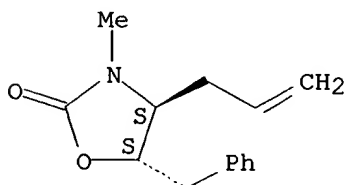
IT 117508-59-5P 117508-60-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and ring cleavage of, amino alc. from)

RN 117508-59-5 HCAPLUS

CN 2-Oxazolidinone, 3-methyl-5-(phenylmethyl)-4-(2-propenyl)-, trans- (9CI)  
(CA INDEX NAME)

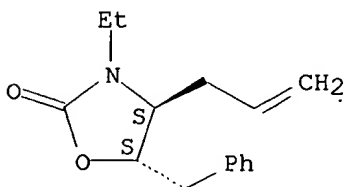
Relative stereochemistry.

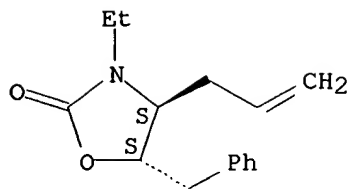


RN 117508-60-8 HCAPLUS

CN 2-Oxazolidinone, 3-ethyl-5-(phenylmethyl)-4-(2-propenyl)-, trans- (9CI)  
(CA INDEX NAME)

Relative stereochemistry.





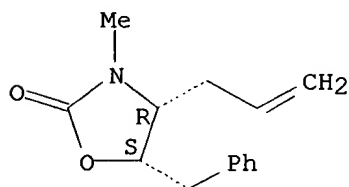
IT 117508-76-6P 117508-77-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 117508-76-6 HCAPLUS

CN 2-Oxazolidinone, 3-methyl-5-(phenylmethyl)-4-(2-propenyl)-, cis- (9CI)  
(CA INDEX NAME)

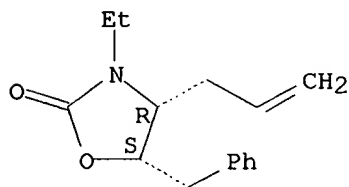
Relative stereochemistry.



RN 117508-77-7 HCAPLUS

CN 2-Oxazolidinone, 3-ethyl-5-(phenylmethyl)-4-(2-propenyl)-, cis- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.



L70 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1983:178457 HCAPLUS

DN 98:178457

TI The intramolecular chemistry of benzyl and phenethyl azidoformates

AU Meth-Cohn, Otto; Patel, Dalpat; Rhouati, Salah

CS Chem. Dep., Univ. Salford, Salford, M5 4WT, UK

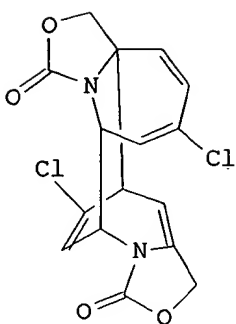
SO Tetrahedron Lett. (1982), 23(48), 5085-8

CODEN: TELEAY; ISSN: 0040-4039

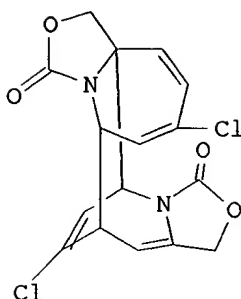
DT Journal

LA English

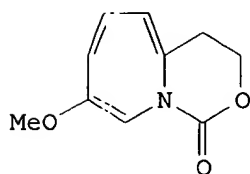
GI



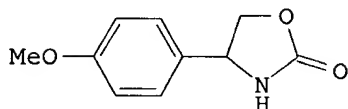
I



II



III



IV

AB Benzyl azidoformates on spray pyrolysis gave, depending on the substituents present, oxazoloazepines, their syn or anti [6 + 4] dimers, their [6 + 6] dimers, benzoxazinones, or aryl isocyanates. 4-ClC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>O<sub>2</sub>CN<sub>3</sub> on pyrolysis at 300.degree. gave a 3:2 mixt. of the syn and anti dimers I and II. Phenylethyl azidoformates on spray pyrolysis gave oxazinoazepines together with, in some cases, 4-aryloxazolidinones. Pyrolysis of 4-MeOC<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>)<sub>2</sub>O<sub>2</sub>CN<sub>3</sub> at 300.degree. gave 61% III and 10% IV.

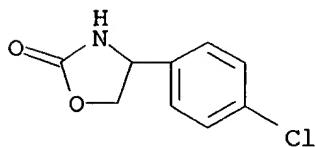
IT 69776-88-1P 69776-92-7P 69776-93-8P

85288-36-4P 85288-37-5P 85288-38-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

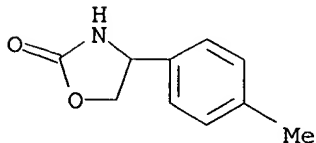
RN 69776-88-1 HCAPLUS

CN 2-Oxazolidinone, 4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



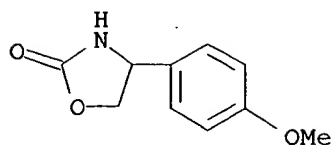
RN 69776-92-7 HCAPLUS

CN 2-Oxazolidinone, 4-(4-methylphenyl)- (9CI) (CA INDEX NAME)



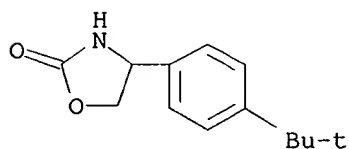
RN 69776-93-8 HCAPLUS

CN 2-Oxazolidinone, 4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



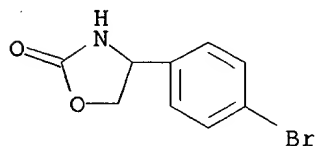
RN 85288-36-4 HCAPLUS

CN 2-Oxazolidinone, 4-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



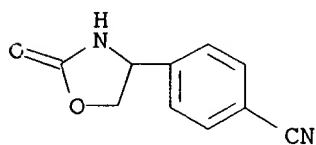
RN 85288-37-5 HCAPLUS

CN 2-Oxazolidinone, 4-(4-bromophenyl)- (9CI) (CA INDEX NAME)



RN 85288-38-6 HCAPLUS

CN Benzonitrile, 4-(2-oxo-4-oxazolidinyl)- (9CI) (CA INDEX NAME)



IT 85288-24-0 85288-25-1 85288-26-2

85288-27-3 85288-28-4 85288-29-5

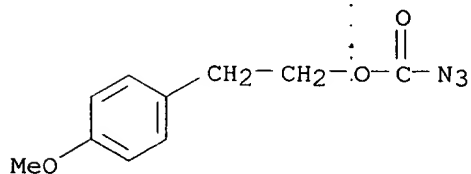
85288-30-8

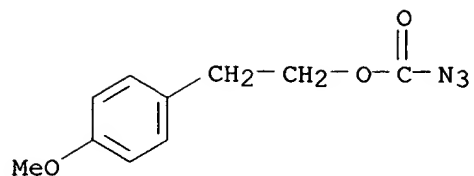
RL: RCT (Reactant)

(pyrolysis of)

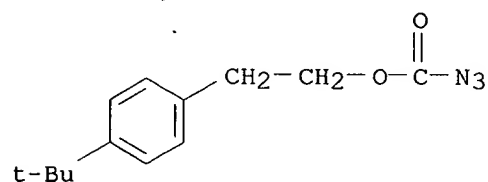
RN 85288-24-0 HCAPLUS

CN Carbonazidic acid, 2-(4-methoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

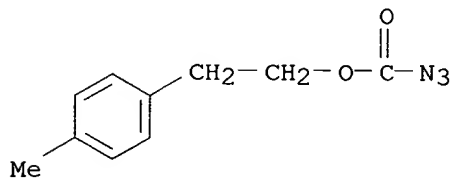




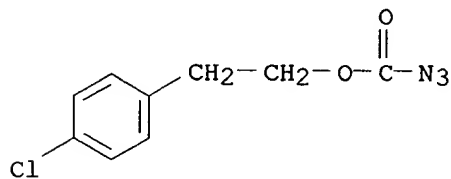
RN 85288-25-1 HCAPLUS  
CN Carbonazidic acid, 2-[4-(1,1-dimethylethyl)phenyl]ethyl ester (9CI) (CA INDEX NAME)



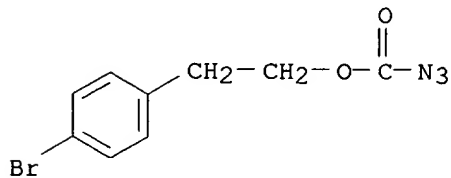
RN 85288-26-2 HCAPLUS  
CN Carbonazidic acid, 2-(4-methylphenyl)ethyl ester (9CI) (CA INDEX NAME)



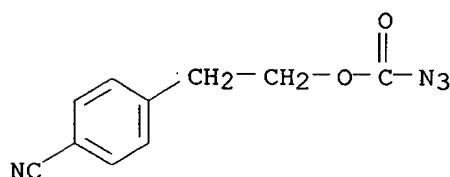
RN 85288-27-3 HCAPLUS  
CN Carbonazidic acid, 2-(4-chlorophenyl)ethyl ester (9CI) (CA INDEX NAME)



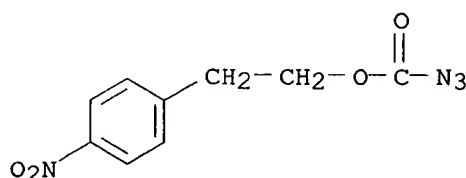
RN 85288-28-4 HCAPLUS  
CN Carbonazidic acid, 2-(4-bromophenyl)ethyl ester (9CI) (CA INDEX NAME)



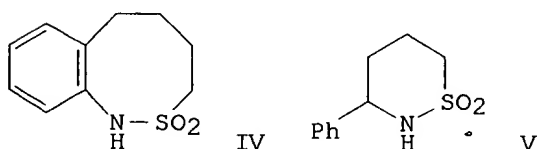
RN 85288-29-5 HCAPLUS  
 CN Carbonazidic acid, 2-(4-cyanophenyl)ethyl ester (9CI) (CA INDEX NAME)



RN 85288-30-8 HCAPLUS  
 CN Carbonazidic acid, 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)



L70 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1982:68493 HCAPLUS  
 DN 96:68493  
 TI Pyrolysis of phenylalkylsulfonyl azides and 2-phenethyl azidoformate.  
 Selectivity of sulfonylnitrenes and contrast between sulfonyl- and  
 carbonylnitrenes  
 AU Abramovitch, Rudolph A.; Hendi, Shivakumar B.; Kress, Albert O.  
 CS Dep. Chem. Geol., Clemson Univ., Clemson, SC, 29631, USA  
 SO J. Chem. Soc., Chem. Commun. (1981), (20), 1087-8  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DT Journal  
 LA English  
 GI



AB Flash vacuum pyrolysis (FVP) and soln. thermolysis of  $\text{Ph}(\text{CH}_2)_n\text{SO}_2\text{N}_3$  (I;  $n = 3-5$ ), and FVP of  $\text{PhCH}_2\text{CH}_2\text{O}_2\text{CN}_3$  (II) were studied. Decompn. of I ( $n = 3$ ) in Freon 113 at 135.degree. for 36 h gave 44% 2,7,8,9-tetrahydrobenzo[1,2-c]thiazepine 1,1-dioxide (III), and FVP at 990.degree. gave 72.4% 1,2,3,4-tetrahydroquinoline. Thermolysis of I ( $n = 4$ ) in Freon 113 at 154.degree. for 36 h gave 30.3% of the sultam IV, whereas FVP at 710.degree. gave 17% sultam V and 7.5% E- $\text{PhCH}_2\text{CH}_2\text{CH}:\text{CHSO}_2\text{NH}_2$ . Thermolysis



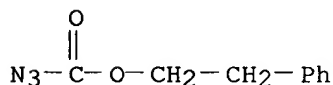
of I (n = 5) in Freon 113 at 154.degree. for 36 h gave 26% 3-benzyl-2,3,4,5,6-pentahydro-1,2-thiazine 1,1-dioxide (VI); FVP at 710.degree. gave 20.3% VI. FVP of II at 650.degree. gave 40% 4-phenyloxazolidinone and 26% tetrahydro-1,3-oxazino[3,4-a]azepin-2-one, but no dihydrocyclopenta[b]pyridine, even at 900.degree..

IT 80639-71-0

RL: RCT (Reactant)  
(flash vacuum pyrolysis of)

RN 80639-71-0 HCAPLUS

CN Carbonazidic acid, 2-phenylethyl ester (9CI) (CA INDEX NAME)

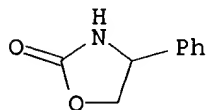


IT 7480-32-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by pyrolysis of phenethyl azidoformate)

RN 7480-32-2 HCAPLUS

CN 2-Oxazolidinone, 4-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L70 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1977:439345 HCAPLUS

DN 87:39345

TI Syntheses of oxazolecarboxylic acid derivatives. XIII. Hydrogenolysis of aminooxazoles. (6). Syntheses and hydrogenolysis of 2-amino-2-oxazolines

AU Tanaka, Chiaki; Ogata, Ikutoshi; Nishida, Motonobu

CS Osaka Coll. Pharm., Osaka, Japan

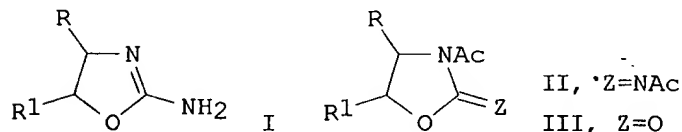
SO Yakugaku Zasshi (1977), 97(2), 157-64

CODEN: YKKZAJ

DT Journal

LA Japanese

GI



AB 2-Amino-2-oxazolines I [R = Ph, R1 = H; R = Ph, R1 = Me (cis and trans); R = Me, R1 = Ph (cis and trans)] were prepd. by the reaction of HOCHR1CHRNH2 with BrCN. Acetylation of I gave the diacetyl derivs. II rather than the monoacetyl derivs. The configuration of I was easily presumed from the

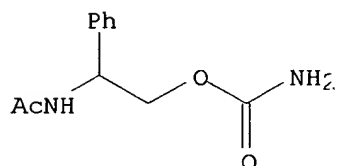
vicinal coupling const. of II. II were hydrolyzed to 3-acetyl-2-oxazolidones III and  $\text{AcNHCO}_2\text{CHR}_1\text{CHRNHAc}$  with 5% HCl at room temp. Catalytic redn. of I (R = Ph) gave the corresponding I (R = cyclohexyl).

IT 63204-94-4P 63204-95-5P 63204-96-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and hydrolysis of)

RN 63204-94-4 HCAPLUS

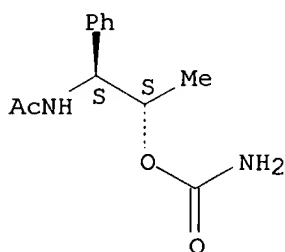
CN Acetamide, N-[2-[(aminocarbonyl)oxy]-1-phenylethyl]- (9CI) (CA INDEX NAME)



RN 63204-95-5 HCAPLUS

CN Acetamide, N-[2-[(aminocarbonyl)oxy]-1-phenylpropyl]-, (R\*,R\*)- (9CI) (CA INDEX NAME)

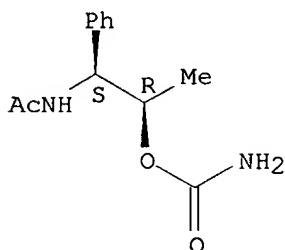
Relative stereochemistry.



RN 63204-96-6 HCAPLUS

CN Acetamide, N-[2-[(aminocarbonyl)oxy]-1-phenylpropyl]-, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

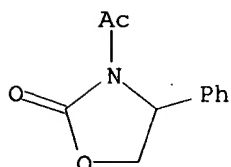


IT 63204-84-2P 63204-85-3P 63204-86-4P

63204-89-7P 63204-90-0P 63204-91-1P

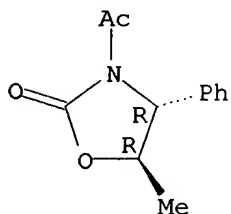
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 63204-84-2 HCAPLUS  
 CN 2-Oxazolidinone, 3-acetyl-4-phenyl- (9CI) (CA INDEX NAME)



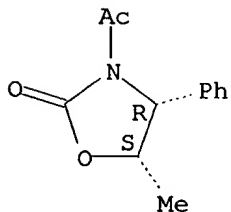
RN 63204-85-3 HCAPLUS  
 CN 2-Oxazolidinone, 3-acetyl-5-methyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

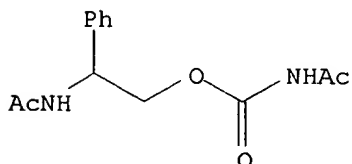


RN 63204-86-4 HCAPLUS  
 CN 2-Oxazolidinone, 3-acetyl-5-methyl-4-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



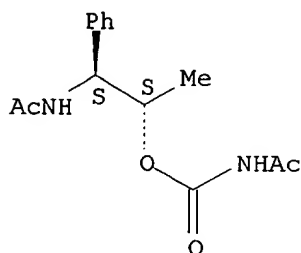
RN 63204-89-7 HCAPLUS  
 CN Carbamic acid, acetyl-, 2-(acetylamino)-2-phenylethyl ester (9CI) (CA INDEX NAME)



RN 63204-90-0 HCAPLUS

CN Carbamic acid, acetyl-, 2-(acetylamino)-1-methyl-2-phenylethyl ester,  
(R\*,R\*)- (9CI) (CA INDEX NAME)

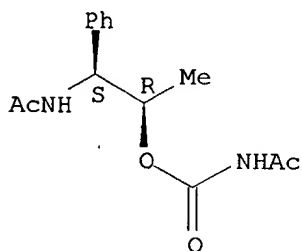
Relative stereochemistry.



RN 63204-91-1 HCAPLUS

CN Carbamic acid, acetyl-, 2-(acetylamino)-1-methyl-2-phenylethyl ester,  
(R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L70 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1972:540025 HCAPLUS

DN 77:140025

TI 4-Aryl-4-oxazolin-2-ones

IN Bottari, Francesco; Saettone, Marco Fabrizio; Tellini, Natale; Serafini,  
Maria Francesca

PA Laboratorio Guidotti e C. S.p.A.

SO Ger. Offen., 15 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2205676	A	19720824	DE 1972-2205676	19720207
	FR 2124468	A5	19720922	FR 1972-3740	19720204
	FR 2124468	B1	19760416		
	SE 370239	B	19741007	SE 1972-1371	19720207
	GB 1386613	A	19750312	GB 1972-5507	19720207
	ES 399572	A1	19741101	ES 1972-399572	19720208
PRAI	IT 1971-45210		19710208		
GI	For diagram(s), see printed CA Issue.				

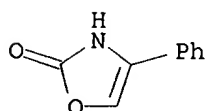
AB Ten title compds. (I, R = Ph, substituted phenyl, 1-, 2-C10H7), useful as muscle relaxants and myotonics, were prepd. by cyclization of RCOCH2O2CNH2 (II). Thus, 40 ml COCl2 (20% in PhMe) was added to 10 g PhCOCH2OH in C6H6-PhMe2 at 0.degree., the mixt. stirred 15 min at room temp., and satd. with NH3(g) at 0.degree. to give 7.55 g II (R = Ph) (III). III (5 g) was refluxed 5 hr in HOAc to give 4.2 g I (R = Ph).

IT 34375-80-9P 34375-81-0P 35961-99-0P  
 35962-00-6P 35962-03-9P 35962-04-0P  
 35962-05-1P 35962-09-5P 35962-10-8P  
 35962-11-9P 35962-12-0P 36404-33-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

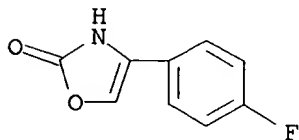
RN 34375-80-9 HCAPLUS

CN 2(3H)-Oxazolone, 4-phenyl- (9CI) (CA INDEX NAME)



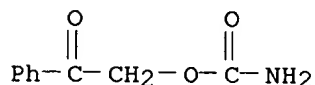
RN 34375-81-0 HCAPLUS

CN 2(3H)-Oxazolone, 4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



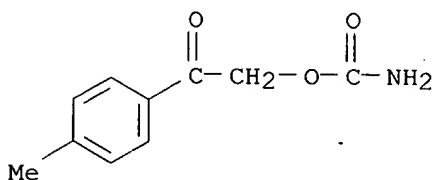
RN 35961-99-0 HCAPLUS

CN Ethanone, 2-[(aminocarbonyl)oxy]-1-phenyl- (9CI) (CA INDEX NAME)



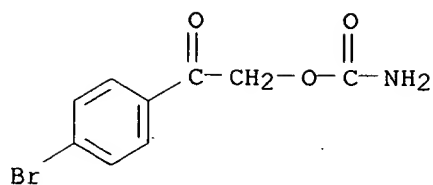
RN 35962-00-6 HCAPLUS

CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-methylphenyl)- (9CI) (CA INDEX NAME)



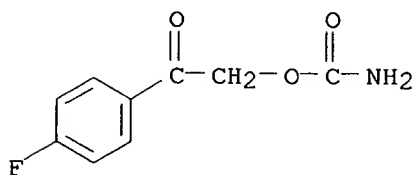
RN 35962-03-9 HCAPLUS

CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-bromophenyl)- (9CI) (CA INDEX NAME)



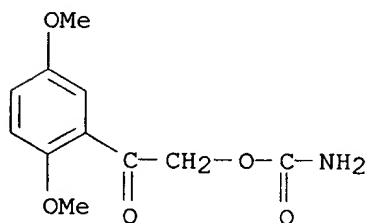
RN 35962-04-0 HCAPLUS

CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



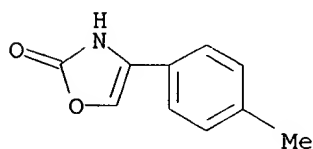
RN 35962-05-1 HCAPLUS

CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



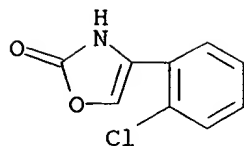
RN 35962-09-5 HCAPLUS

CN 2(3H)-Oxazolone, 4-(4-methylphenyl)- (9CI) (CA INDEX NAME)

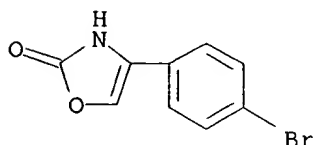


RN 35962-10-8 HCAPLUS

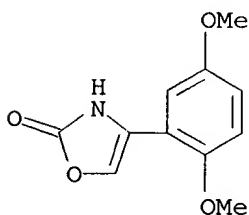
CN 2(3H)-Oxazolone, 4-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



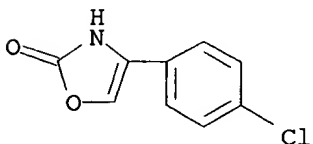
RN 35962-11-9 HCAPLUS  
 CN 2(3H)-Oxazolone, 4-(4-bromophenyl)- (9CI) (CA INDEX NAME)



RN 35962-12-0 HCAPLUS  
 CN 2(3H)-Oxazolone, 4-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 36404-33-8 HCAPLUS  
 CN 2(3H)-Oxazolone, 4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



L70 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1972:108224 HCAPLUS  
 DN 76:108224  
 TI Synthesis and biological activity of some 4-aryl-substituted  
 4-oxazolin-2-ones  
 AU Bottari, Francesco; Nannipieri, Enrico; Saettone, Marco F.; Serafini,  
 Maria F.  
 CS Pharm. Chem. Inst., Univ. Pisa, Pisa, Italy  
 SO J. Med. Chem. (1972), 15(1), 39-42  
 CODEN: JMCMAR  
 DT Journal  
 LA English  
 AB Of a series of 4-aryl-substituted 4-oxazolin-2-ones, some (group 1)

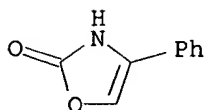
produced myotonic symptoms and antagonized barbiturate-induced sleep at dose levels of 30-100 mg/kg i.p. in mice, whereas others (group 2) showed muscle relaxant and sedative activity. Group 1 included 4-phenyl-4-oxazolin-2-one (I) [34375-80-9] and 4-(p-fluorophenyl)-4-oxazolin-2-one [34375-81-0], and group 2 included the 4-(p-biphenyl) and 4-(2-naphthyl) derivs. (III, IV). I was obtained from the relaxant drug, 2-hydroxy-2-phenylethyl carbamate (styramate) [94-35-9], through oxidn. and cyclization; the other compds. were prepd. similarly.

IT 34375-80-9 34375-81-0 35962-09-5  
35962-10-8 35962-11-9 35962-12-0  
36404-33-8

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pharmacology of)

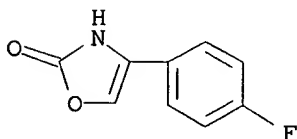
RN 34375-80-9 HCAPLUS

CN 2(3H)-Oxazolone, 4-phenyl- (9CI) (CA INDEX NAME)



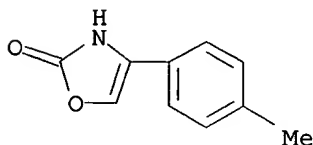
RN 34375-81-0 HCAPLUS

CN 2(3H)-Oxazolone, 4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



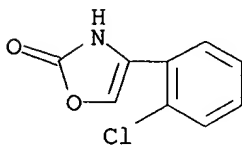
RN 35962-09-5 HCAPLUS

CN 2(3H)-Oxazolone, 4-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 35962-10-8 HCAPLUS

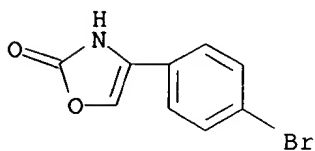
CN 2(3H)-Oxazolone, 4-(2-chlorophenyl)- (9CI) (CA INDEX NAME)





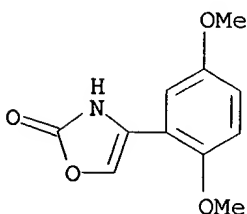
RN 35962-11-9 HCAPLUS

CN 2(3H)-Oxazolone, 4-(4-bromophenyl)- (9CI) (CA INDEX NAME)



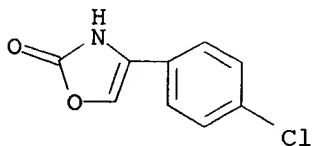
RN 35962-12-0 HCAPLUS

CN 2(3H)-Oxazolone, 4-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 36404-33-8 HCAPLUS

CN 2(3H)-Oxazolone, 4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



IT 35961-99-0P 35962-00-6P 35962-01-7P

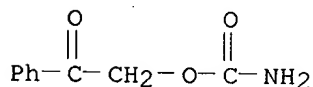
35962-02-8P 35962-03-9P 35962-04-0P

35962-05-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

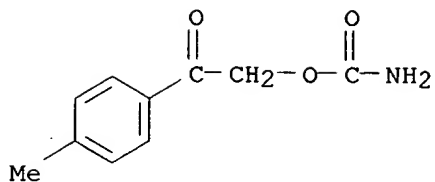
RN 35961-99-0 HCAPLUS

CN Ethanone, 2-[(aminocarbonyl)oxy]-1-phenyl- (9CI) (CA INDEX NAME)

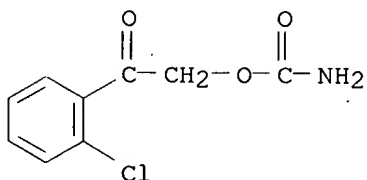


RN 35962-00-6 HCAPLUS

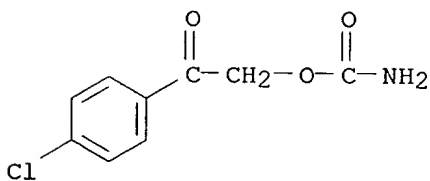
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-methylphenyl)- (9CI) (CA INDEX NAME)



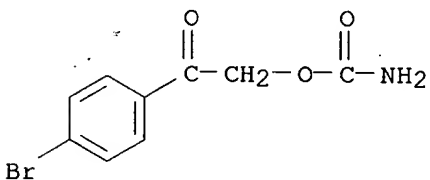
RN 35962-01-7 HCAPLUS  
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



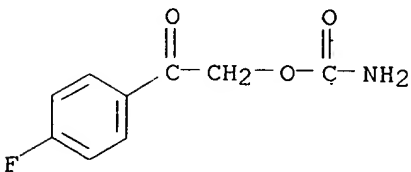
RN 35962-02-8 HCAPLUS  
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

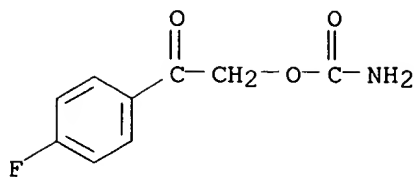


RN 35962-03-9 HCAPLUS  
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-bromophenyl)- (9CI) (CA INDEX NAME)

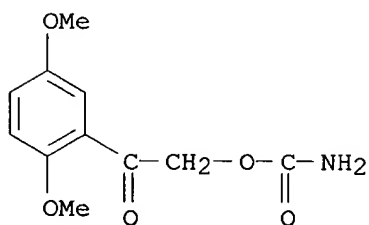


RN 35962-04-0 HCAPLUS  
CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

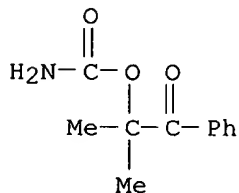




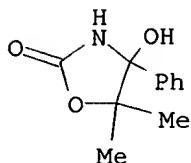
RN 35962-05-1 HCAPLUS  
 CN Ethanone, 2-[(aminocarbonyl)oxy]-1-(2,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



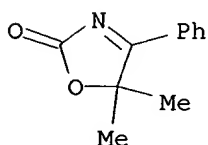
L70 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2001 ACS  
 AN 1971:488520 HCAPLUS  
 DN 75:88520  
 TI Synthesis and properties of 3-oxazol-2-ones  
 AU Hofmann, Hans; Wagner, Ruediger; Uhl, Juergen  
 CS Inst. Org. Chem., Univ. Erlangen-Nuernberg, Erlangen, Ger.  
 SO Chem. Ber. (1971), 104(7), 2134-42  
 CODEN: CHBEAM  
 DT Journal  
 LA German  
 GI For diagram(s), see printed CA Issue.  
 AB RCOCr1R2OH (I), where R, R1R2 = Ph, tert-Bu, or Me or R-R2 = (CH2)5, reacted with ClSO2NCO to give RCOCr1R2O2CNH2 (II), sometimes in mixts. with the isomeric 4-hydroxyoxazolidin-2-ones. Subsequent thermal cyclization led to the corresponding 3-oxazolin-2-ones (III), which on LiAlH4 redn. yielded the oxazolidin-2-ones (IV). Alk. sapon. of IV gave I.  
 IT 33664-82-3P 33664-83-4P 33664-90-3P  
 33664-93-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)  
 RN 33664-82-3 HCAPLUS  
 CN Propiophenone, 2-hydroxy-2-methyl-, carbamate (8CI) (CA INDEX NAME)



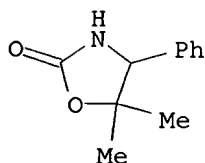
RN 33664-83-4 HCAPLUS  
 CN 2-Oxazolidinone, 4-hydroxy-5,5-dimethyl-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 33664-90-3 HCAPLUS  
 CN 2(5H)-Oxazolone, 5,5-dimethyl-4-phenyl- (9CI) (CA INDEX NAME)



RN 33664-93-6 HCAPLUS  
 CN 2-Oxazolidinone, 5,5-dimethyl-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



L70 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1969:36863 HCAPLUS

DN 70:36863

TI Stereochemical studies. II. Thermal and photochemical decompositions of optically active alkyl azidoformates

AU Terashima, Shiro; Yamada, Shunichi

CS Fac. Pharm. Sci., Univ. Tokyo, Tokyo, Japan

SO Chem. Pharm. Bull. (Tokyo) (1968), 16(10), 1953-71

CODEN: CPBTAL

DT Journal

LA English

AB The thermal and photochem. decompns. of three types of optically active alkyl azidoformates (I) were attempted, and it was found in both cases, that optically active 2-oxazolidinones (II) were obtained with nearly complete retention of configuration. The yield of II was very low (5%) in the thermal decompn. and moderate (25-30%) in the photochem. one. Considering the relation between stereospecificity and spin multiplicity of alkoxy carbonyl nitrene, a mechanism was proposed suggesting that the singlet state alkoxy carbonyl nitrene generated from I, either by heating or by irradiation, was inserted into the intramolecular optically active C-H bond

through an insertion transition state. Moreover, in the course of these studies, the abs. configuration of .alpha.-methylphenylglycine (2-amino-2-phenylpropionic acid) was detd. using thermal decompn. Preliminary expts. using racemic compds. were also reported.

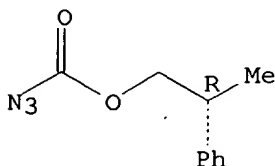
IT 13398-27-1 22436-12-0

RL: RCT (Reactant)  
(photolysis of)

RN 13398-27-1 HCAPLUS

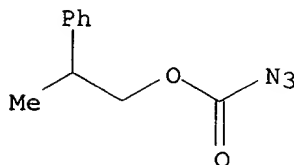
CN Formic acid, azido-, .beta.-methylphenethyl ester, (R)-(+)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 22436-12-0 HCAPLUS

CN Carbonazidic acid, 2-phenylpropyl ester (9CI) (CA INDEX NAME)



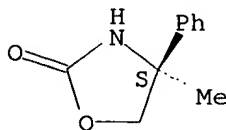
IT 13398-55-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 13398-55-5 HCAPLUS

CN 2-Oxazolidinone, 4-methyl-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L70 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2001 ACS

AN 1967:94936 HCAPLUS

DN 66:94936

TI Carbamates. IV. Cyclization of N-substituted phenacyl carbamates to 4-hydroxyoxazolidin-2-ones and 4-oxazolin-2-ones

AU Saettone, Marco F.; Nuti, Vittorio; Da Settimo, Antonio

CS Inst. Chim. Farm., Univ. Pisa, Pisa, Italy

SO Gazz. Chim. Ital. (1966), 96(11), 1615-29

CODEN: GCITA9

DT Journal

LA Italian

GI For diagram(s), see printed CA Issue.

AB cf. CA 64, 19457f. Phenacyl alc. (6.12 g.) in 80 ml. C<sub>6</sub>H<sub>6</sub> and 10 ml. PhNMe<sub>2</sub> is treated at 0.degree. with 25 ml. 20% COCl<sub>2</sub>(PhMe) to give 32% phenacyl N-methylcarbamate (I), m. 106-7.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine). Similarly prepd. are the following compds. of the general formula BzCH<sub>2</sub>O<sub>2</sub>CNHR (II) (R, m.p., and % yield given): Et, 105-6.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine), 37; iso-Pr, 112-13.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine), 55; iso-Bu, 98-100.degree. (EtOH), 50; tert-Bu, 80-1.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine), 44; allyl, 88-9.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine), 30; cyclopropyl, 149-51.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine), 53; cyclopentyl, 129-30.degree. (EtOAc-ligroine), 66; cyclohexyl, 153-4.degree. (EtOAc-ligroine), 58; p-MeOC<sub>6</sub>H<sub>4</sub>, 158-9.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine), 69. The II are refluxed with Et<sub>3</sub>N to give 4-hydroxyoxazolidin-2-ones of the general formula III and the III are refluxed with HOAc to give 4-phenyl-4-oxazolin-2-ones of the general formula IV. Thus, a soln. of 4 g. II (R = iso-Bu) in 5 ml. EtOH and 0.5 ml. Et<sub>3</sub>N is refluxed 4 hrs. to give 60% 3-isobutyl-4-phenyl-4-hydroxyoxazolidin-2-one, m. 120-3.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine). Similarly prepd. are the following III (R and m.p. given): Me, 146-8.degree. (EtOH); Et, 104-5.degree. (EtOH); iso-Pr, 154-6.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine); allyl, 110-11.degree. (EtOH-water); cyclopropyl, 140-2.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine). A soln. of 2 g. I in 15 ml. HOAc is refluxed 8 hrs. to give 94% 4-phenyl-3-methyl-4-oxazolin-2-one, m. 85-6.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine). Similarly prepd. are the following IV (R, m.p., and % yield given): iso-Pr, 83-4.degree. (ligroine), 81; iso-Bu, -, -; tert-Bu, 122-3.degree. (EtOH), 10.8; allyl, 43-6.degree. (EtOH-water), 50; cyclopropyl, 65-6.degree. (EtOH-water), 52; cyclopentyl, 112-13.degree. (EtOH), 60; cyclohexyl, 99-100.degree. (C<sub>6</sub>H<sub>6</sub>-ligroine), 70; p-MeOC<sub>6</sub>H<sub>4</sub>, 135-6.degree. (EtOH), 85. A soln. of 6.12 g. BzCH<sub>2</sub>OH in 80 ml. C<sub>6</sub>H<sub>6</sub> and 10 ml. pyridine is treated at 0.degree. with 25 ml. 20% COCl<sub>2</sub>(PhMe) and the mixt. is agitated 1 hr. at 0.degree. to give 50% bis(phenacyl) carbonate, m. 116-16.5.degree. (C<sub>6</sub>H<sub>6</sub>). IV (R = cyclohexyl) shows antidepressant activity in mice at 300 mg./kg.; III (R = tert-Bu) and IV (R = iso-Pr) demonstrate fungicidal activity.

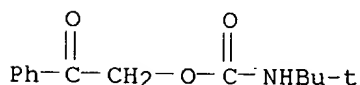
IT 13098-02-7P 13098-04-9P 13098-05-0P

13626-63-6P 13626-64-7P 13626-67-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and cyclization of)

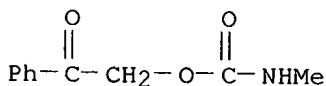
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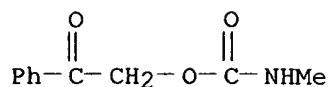
CN Carbamic acid, (1,1-dimethylethyl)-, 2-oxo-2-phenylethyl ester (9CI) (CA INDEX NAME)



RN 13098-04-9 HCAPLUS

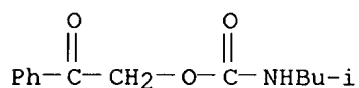
CN Ethanone, 2-[[[methylamino)carbonyl]oxy]-1-phenyl- (9CI) (CA INDEX NAME)





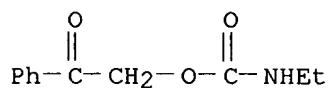
RN 13098-05-0 HCAPLUS

CN Carbamic acid, (2-methylpropyl)-, 2-oxo-2-phenylethyl ester (9CI) (CA INDEX NAME)



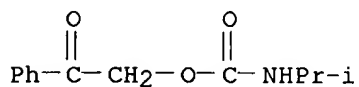
RN 13626-63-6 HCAPLUS

CN Carbamic acid, ethyl-, ester with 2-hydroxyacetophenone (8CI) (CA INDEX NAME)



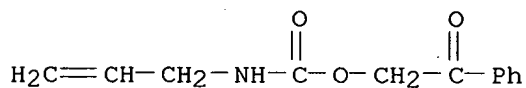
RN 13626-64-7 HCAPLUS

CN Carbamic acid, (1-methylethyl)-, 2-oxo-2-phenylethyl ester (9CI) (CA INDEX NAME)



RN 13626-67-0 HCAPLUS

CN Carbamic acid, allyl-, ester with 2-hydroxyacetophenone (8CI) (CA INDEX NAME)



IT 13098-03-8P 13098-06-1P 13098-07-2P

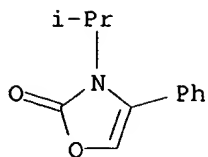
13626-72-7P 13626-73-8P 13626-74-9P

13626-76-1P 13626-78-3P 13626-79-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

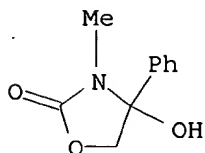
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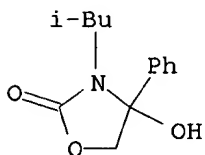
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CN 2-Oxazolidinone, 4-hydroxy-3-methyl-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



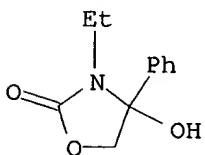
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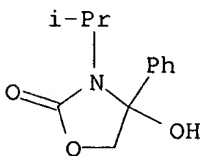
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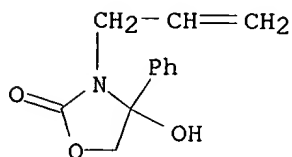
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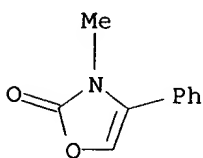
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CN 2-Oxazolidinone, 3-allyl-4-hydroxy-4-phenyl- (8CI) (CA INDEX NAME)



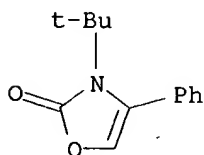
RN 13626-76-1 HCAPLUS

CN 4-Oxazolin-2-one, 3-methyl-4-phenyl- (8CI) (CA INDEX NAME)



RN 13626-78-3 HCAPLUS

CN 4-Oxazolin-2-one, 3-tert-butyl-4-phenyl- (8CI) (CA INDEX NAME)



RN 13626-79-4 HCAPLUS

CN 4-Oxazolin-2-one, 3-allyl-4-phenyl- (8CI) (CA INDEX NAME)

